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ABSTRACT

Molecular diffusion and electrochemical migration are important processes affecting transport of charged species in porous media. In this work, we present a two-dimensional multicomponent reactive transport model taking into account the electrostatic interactions during transport of charged species in physically and chemically heterogeneous domains [1]. The modeling approach is based on the Nernst-Planck formulation and on the description of compound-specific and spatially variable diffusive/dispersive fluxes. The multicomponent ionic transport code is coupled with the geochemical code PHREEQC by utilizing the IPhreeqc module [2], thus enabling to perform the geochemical calculations included in the PHREEQC's reaction package. The multicomponent reactive transport code is benchmarked by comparing the model outcomes with the high-resolution experimental datasets obtained from controlled laboratory flow-through experiments. The experiments were performed in a quasi two-dimensional bench-scale setup, packed with water-saturated porous media, using dilute solutions of different strong electrolytes. The experimental results showed a remarkable influence of the charge interactions between the ionic species also in advection-dominated flow regimes [3]. The excellent agreement between the experimental results and the model simulations validates the proposed charge coupled diffusion/dispersion and electromigration calculations for macroscopic transport of charged species in porous media. Furthermore, we validated the 2-D multicomponent reactive transport code against 1-D PHREEQC simulations and we used the model to explore the effects of charge interactions in reactive transport scenarios in physically and chemically heterogeneous porous media.

REFERENCES

[1] Muniruzzaman M and Rolle M (2016). Adv. Water Resour. 98, 1-15.
[2] Charlton SR and Parkhurst DL (2011). Comput. Geosci. 37, 1653–1663.
[3] Rolle M, Muniruzzaman M, Haberer CM, Grathwohl P (2013). Geochim. Cosmochim. Acta 120, 195-205.

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